

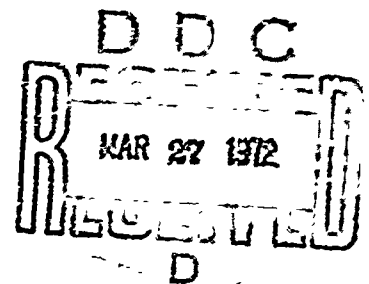
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AIR FORCE CAMBRIDGE RESEARCH LABORATORIES
L. G. HANCOCK FIELD, BEDFORD, MASSACHUSETTS

Photo-Equilibrium of Barium

GORDON T. BEST
VICTOR L. CORBIN



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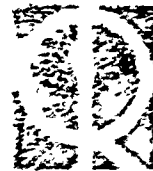
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Abstract

A model for numerical simulation of the solar pumping of a simple atomic system is constructed and compared with the exact analytical solution. The process is then extended to cover the more complex 5-level 5-transition barium ion term scheme, and the 61-level 86-transition barium neutral term scheme. An advantage of the stepwise simulation is that in addition to yielding the equilibrium relative level populations and transition intensities, it also permits the dynamic grow-in to equilibrium to be studied. The neutral barium system has also been studied with the inclusion of photoionization from each of several metastable levels.

Contents

1. INTRODUCTION	1
2. ANALYSIS OF SIMPLE 3-LEVEL SYSTEM	4
2.1 Exact Analytical Solution	4
2.2 Approximate Analytical Solution	6
2.3 Computed Stepwise Solution	7
3. BARIUM ION SYSTEM	9
4. BARIUM NEUTRAL SYSTEM	10
4.1 Equilibrium Without Photoionization	10
4.2 Readjustment of Equilibrium After Sudden Removal of Some Metastable Atoms	16
4.3 Photoionization From $1,^3D$ -Metastable Levels	16
REFERENCES	21
APPENDIX A	23

Illustrations

1. Simple Term Diagram for Hypothetical $C_{2\lambda}$	4
2. Barium Ion Term Diagram	10
3. Barium Neutral Term Diagram	11
4. Populations as a Function of Time	14

Tables

1. Input Data for Barium, Neutral System	12
2. Equilibrium Emission Line Intensities per Barium Atom, Without Ionization	15
3. Data Yielding Metastable Photoionization Time Constant of Required Magnitude	17

Photo-Equilibrium of Barium

1. INTRODUCTION

When a cloud of atom (or ion) vapor is irradiated by sunlight, the relative populations of the energy levels and the relative intensities of the optical transitions are determined by: (1) the oscillator strengths of the transitions, and (2) the relative intensities of sunlight at the wavelengths of these transitions. In the case of barium ion, there are 5 levels and 5 permitted transitions; the equilibrium solution when all transitions have negligible optical thickness, has already been given by Best (1968).

If we number the energy levels of a term scheme from 1 to N , starting with the ground state, then the rate of change of population P_n of level n due to absorption of solar photons by lower-lying energy levels is equal to

$$\frac{dP_n}{dt} = \sum_{m=1}^{n-1} 0.02654 P_m \theta_{nm} f_{mn} \text{sec}^{-1} \quad (1)$$

where P_m is the population of the m^{th} level, θ_{nm} is the solar irradiance (photons $\text{cm}^{-2} \text{sec}^{-1} \text{Hz}^{-1}$) at the wavelength λ_{nm} of the transition, and f_{mn} is the oscillator strength of the transition. The rate of depopulation of level n due to

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photon absorption to higher energy levels is equal to

$$\frac{dP_n}{dt} = - \sum_{m=n+1}^N 0.02654 P_n \theta_{mn} f_{nm} \text{sec}^{-1}. \quad (2)$$

The rate of population of level n due to photon emission by higher energy levels is equal to

$$\frac{dP_n}{dt} = \sum_{m=n+1}^N P_m A_{mn} \text{sec}^{-1}. \quad (3)$$

In Eq. (3), A_{mn} (Einstein radiative transition probability) is equal to

$$A_{mn} = \frac{g_n}{g_m} \cdot 66698 \times 10^{16} f_{nm} \lambda_{mn}^{-2}. \quad (4)$$

The rate of depopulation of level n due to photon emission to lower energy levels is equal to

$$\frac{dP_n}{dt} = - \sum_{m=1}^{n-1} P_n A_{nm}. \quad (5)$$

At equilibrium the arithmetic sum of the rates of population and depopulation due to the above four processes is, of course, zero and we obtain for each of the N levels an equation of the form:

$$\begin{aligned} \sum_{m=1}^{n-1} (0.02654 P_m \theta_{nm} f_{mn} - P_n A_{nm}) \\ - \sum_{m=n+1}^N (0.02654 P_n \theta_{mn} f_{nm} - P_m A_{mn}) = 0. \end{aligned} \quad (6)$$

By numerically evaluating the coefficients of P_m and P_n in Eq. (6), we obtain a set of N simultaneous equations of the form

$$\sum_{m=1}^N a_{nm} P_m = 0. \quad (7)$$

If we include the additional constraint that $\sum_{m=1}^N P_m = 1$, the solution is obtained by the inversion of a square matrix of dimension $N-1$.

In the case of barium ion where there are only 5 transitions for a 5-level term scheme, many of the elements are zero and it is not necessary to perform the matrix inversion in order to solve for equilibrium conditions. However, for neutral barium there are 62 possible energy levels (if we include the ionization limit), and the inversion of a 61×61 matrix presents problems even with a large computer. In addition since there are 86 permitted transitions, all but 172 of the 61^2 elements of the matrix will be zero, and the program would spend a considerable amount of computer time manipulating quantities of zero magnitude.

In addition, because of the interest in the dynamic properties of the problem (the time it takes to grow in to equilibrium of the ion radiations, the time constant for significant pumping of the $1, 3D$ metastable levels of neutral barium, the possible sensitivity of relative intensities to the identity of the ion precursor), it seemed that a stepwise solution to the problem would be more informative. In this approach, it is initially assumed that all species are in the ground state. The sun is allowed to shine for a small time δt , during which a certain population of excited states is built up, depending on the solar irradiance and the values of the oscillator strengths of the permitted transitions. Then the sun is "turned off" and the excited states are permitted to radiate, thereby adding to the population of certain lower levels. By properly choosing the value of the time interval, the result will be a good approximation to the situation existing at the end of the period δt . The process is then allowed to repeat, using the new relative populations of each of the energy levels as a starting point. It was intuitively felt that the correct choice of the value of δt was properly made when it had a value somewhat greater than the lifetime of the excited state (that is, 10^{-6} sec for weak transitions), and somewhat less than the lifetime of metastable levels. Although the radiative lifetime of metastable levels may be measured in seconds or tens of seconds, in practice the actual lifetime is more likely to be of the order of one second due to the absorption of solar photons.

Initially δt was chosen as 10^{-3} sec, and it was later increased to 10^{-2} sec without significantly changing the results (when examined with time resolution of 0.1 sec or greater).

In order to check on the validity of the method a simple model, which could also be solved analytically, was constructed and evaluated by both techniques. The solution of a 2-level 1-transition scheme is trivial and would not permit an evaluation of the technique. Therefore, a 3-level 2-transition scheme with one metastable level was chosen for analysis.

2. ANALYSIS OF SIMPLE 3-LEVEL SYSTEM

2.1 Exact Analytical Solution

Figure 1 shows the simple term scheme and permitted transitions. The solar irradiances were chosen so that the rate of population of level 3 from level 1 would be $1 \times P_1 \text{ sec}^{-1}$, and the rate of upward pumping from level 2 to level 3 was $0.2 \times P_2 \text{ sec}^{-1}$. In addition we allowed

$$A_{32} = 10^8 \text{ sec}^{-1}$$

$$A_{31} = 2 \times 10^8 \text{ sec}^{-1}$$

The equations governing radiative equilibrium of this situation are

$$\frac{dP_1}{dt} = -aP_1 + bP_3 \quad 8(a)$$

$$\frac{dP_2}{dt} = -cP_2 + dP_3 \quad 8(b)$$

$$\frac{dP_3}{dt} = aP_1 + cP_2 - (b+d)P_3 \quad 8(c)$$

and

$$\sum_n P_n = 1$$

where

$$a = 1.0$$

$$b = 2 \times 10^8$$

$$c = 0.2$$

$$d = 1 \times 10^8$$

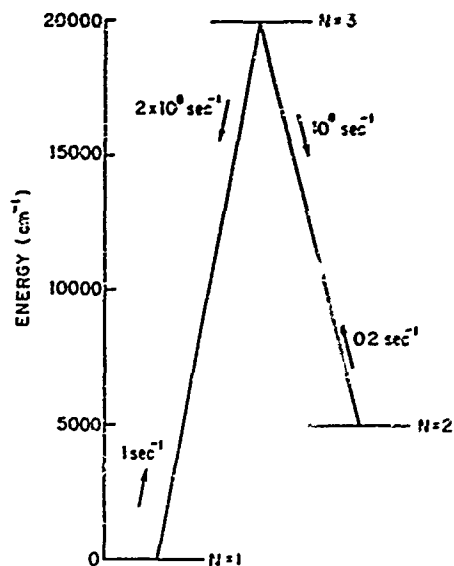


Figure 1. Simple Term Diagram for Hypothetical Case

The exact solution of Eqs. (1) has been performed by Qureshi (1971). For the particular case where the initial conditions are at $t=0$, $P_1 = 1$, $P_2 = P_3 = 0$, the solution is

$$P_1 = \frac{bc}{a^2 - \beta^2} [1 - f(t)] + g(t) + (b+cd)h(t) \quad (9a)$$

$$P_2 = \frac{ad}{a^2 - \beta^2} [1 - f(t)] \quad (9b)$$

$$P_3 = \frac{ac}{a^2 - \beta^2} [1 - f(t)] + ah(t) \quad (9c)$$

where

$$a^2 - \beta^2 = ac + ad + bc$$

$$a = \frac{1}{2} (a + b + c + d)$$

$$\beta = \sqrt{a^2 - (ac + ad + bc)}$$

and where

$$f(t) = e^{-at} \left(\cosh \beta t + \frac{a}{\beta} \sinh \beta t \right) \quad (10a)$$

$$g(t) = e^{-at} \left(\cosh \beta t - \frac{a}{\beta} \sinh \beta t \right) \quad (10b)$$

$$h(t) = e^{-at} \left(\frac{\sinh \beta t}{\beta} \right) \quad (10c)$$

We may also rewrite Eq. (10) as

$$f(t) = \frac{1}{2} e^{-at} \left[\left(1 + \frac{a}{\beta}\right) e^{\beta t} + \left(1 - \frac{a}{\beta}\right) e^{-\beta t} \right] \quad (11a)$$

$$g(t) = \frac{1}{2} e^{-at} \left[\left(1 - \frac{a}{\beta}\right) e^{\beta t} + \left(1 + \frac{a}{\beta}\right) e^{-\beta t} \right] \quad (11b)$$

$$h(t) = \frac{1}{2\beta} e^{-at} \left[e^{\beta t} - e^{-\beta t} \right] \quad (11c)$$

Thus

$$P_1 = \frac{P_1}{\alpha^2 - \beta^2} + \frac{P_1}{\alpha^2} e^{-\alpha t} \left[\frac{-\alpha}{\alpha^2 - \beta^2} + (\alpha - \beta) + (\alpha + \beta) \right] \\ + \frac{P_1}{\beta^2} e^{-\beta t} \left[\frac{-\beta}{\alpha^2 - \beta^2} + (\alpha + \beta) - (\alpha - \beta) \right]$$

Inserting values for α , β , c and d we find

$$\alpha = 1.5 \times 10^8 + 0.6$$

$$\beta = 1.5 \times 10^8 + 0.1333$$

$$\alpha^2 - \beta^2 = 1.4 \times 10^8 + 0.2$$

$$\beta^2 = 0.5 \times 10^8$$

$$(c+d) = 3 \times 10^8 + 0.2$$

and

$$P_1 = 0.2857 + e^{-0.4666t} [0.7143 - 0.003 \times 10^{-3}] \\ + e^{-3 \times 10^8 t} [0.1777 \times 10^{-2}].$$

Obviously for times greater than 10^{-8} sec, the third term is negligible and we may write the solution as

$$P_1 = 0.2857 + e^{-0.4666t} [0.7143] . \quad (12)$$

2.2 Approximate analytical solution

It appeared that an approximate analytical solution for this model might be possible on the basis of the following argument:

Of the atoms excited to level 3, two-thirds will decay to level 1, and one-third to level 2. Then Eqs. (3) become, with the appropriate numerical coefficients,

$$\frac{dP_1}{dt} = -(1 + P_1) \frac{1}{\tau_1} + (0.2 P_2) \frac{2}{3} \quad 13(a)$$

$$\frac{dP_2}{dt} = - (0.2 P_2)^{2/3} + (1 \times P_1)^{1/3} . \quad 13(b)$$

Solving these and putting the initial conditions as $P_1 = 1$, $P_2 = 0$, we obtain

$$P_1 = 0.2857 + 0.7143 \exp(-0.4666t) \quad 14(a)$$

$$P_2 = 0.7143 [1 - \exp(-0.4666t)] . \quad 14(b)$$

Note that the solution Eq. (14a) is identical with that obtained as Eq. (12). Thus this approximation is valid for all but the first microsecond or so, and it is therefore possible for: (1) the solution to the dynamic grow-in to equilibrium of the barium ion to be derived as the solution of 3 (rather than 5) coupled linear differential equations; and for (2) the corresponding neutral barium process to be obtained as the solution of a set of 8 (rather than 61) equations.

The function Eq. (14a) has been evaluated by hand (using a Wang program-mable calculator) and gives excellent agreement (at 0.1 sec intervals) with the computed stepwise solution (to be described below).

Note that the time constant for pumping of the metastable level is 2.143 sec, whereas the simple approach used earlier (Best et al, 1970) to give the rate of pumping of BaI^1D would yield an expected time constant of 3 sec. Consequently, it may be inferred that the rate estimated by Best et al (1970) for BaI^1D pumping may be inaccurate by as much as 30 percent; that is, it could be somewhat less than the 1.24 sec derived.

2.3 Computed Stepwise Solution

A computer program has been written for the general case of energy levels in the range $1 \leq N \leq NMAX$ and associated optical transitions $1 \leq L \leq LMAX$. In this we assume initially that all the population resides in the ground state $N = 1$. As noted in the introduction above, the computation interval DELTC was allowed to be greater than the lifetime of the excited states, but less than the time between optical excitations from the ground or metastable levels. This model was allowed to be pumped by the solar irradiation with DELTC = 0.01 sec. Since this was a test of the general program, a brief qualitative description is given here.

Input data consists of:

- NMAX : the maximum number of energy levels
- LMAX : the maximum number of optical transitions
- DE LTC : the computation time interval
- NMIN : the number of stable (or metastable) levels

For each of the energy levels we read in:

N : the sequential number
 E(N) : the energy in cm^{-1}
 G(N) : the statistical weight

For each of the optical transitions we read in:

L : the sequential number
 WVL(L) : the wavelength in Angstroms
 NU(L) : the upper energy level number
 NL(L) : the lower energy level number
 F(L) : the transition oscillator strength
 SINC(L) : the solar continuum irradiance
 FLD(L) : the Fraunhofer line depth

The program initially checks the above data for accuracy by computing the wavelength of each transition for the energy level numbers of the upper and lower states, and then comparing with the input data; correction to wavelength in air is made above 2460\AA . This wavelength is used so as to permit comparison with the data tabulated by Miles et al (1969).

Initial populations are all set equal to zero, with the exception of $P(1) = 1.0$. The rates of population of each of the upper levels from each of the lower levels are computed in turn for DELTC, and after all LMAX transitions have been considered corresponding changes in upper and lower energy level populations are made. If I is the solar continuum irradiance in $\text{watts m}^{-2} \text{nm}^{-1}$ and λ_μ is the wavelength in microns, then

$$\theta = 1679.4 \lambda_\mu^3 I \quad (15)$$

and the rate of pumping of the upper level NU from the lower level NL is

$$\frac{dP(NU)}{dt} = 0.02654 P(NL) \theta f \text{ FLD} . \quad (16)$$

Then the system is permitted to radiate, and the branching ratios are computed in terms of the computed Einstein A coefficients:

$$AE = \frac{G(NL)}{G(NU)} 0.66698 \times 10^8 f \lambda_\mu^{-2} . \quad (17)$$

Since all lifetimes are much less than DELTC, we perform a check to ensure that all levels with $N > N_{\text{MIN}}$ have emptied. The emptying process for each level is in accordance with computed branching ratios. Printout and plotting of data is called

for at meaningful intervals. This data includes populations of all stable (or metastable) levels and the brightnesses of emission lines.

In the case of this synthetic model, values of the input parameters were chosen to match the input data of paragraph 2. 1:

N	$\bar{E}(N)$	$G(N)$
1	0	4
2	5000	4
3	20,000	2

and

L	$WVL(L)$	$F(L)$	$SINC(L)$	$FLD(L)$
1	4998.60	0.375	0.959	0.500
2	6664.83	0.333	0.455	0.100

The computer tabulated output agreed exactly with the analytical function computed according to Eq. (14a).

3. BARIUM ION SYSTEM

The program providing the stepwise solution to the optically thin radiative transport problem was next applied to the barium ion system with 5 levels and 5 transitions (Figure 2). This allowed the equilibrium value to be compared with that calculated earlier (Best, 1968), as a further check on the program.

At equilibrium the values obtained were:

N	$E(\text{cm}^{-1})$	$P(N)$	$P(N)^*$
1	0	0.575	0.575
2	4873.85	0.130	0.130
3	5674.82	0.294	0.294
4	20261.6		
5	21952.4		
L	$WVL(\text{\AA})$	$BR(N)$	$BR(N)^*_+$
1	4554.03	0.780	0.780
2	4934.09	0.299	0.299
3	5854.68	0.032	0.032
4	6141.72	0.243	0.243
5	6496.90	0.103	0.103

* Values (per total ion) given in Best (1968).

+ Dr. J. H. M. Fu (EG&G) has kindly pointed out a typographical error in Table II of Best (1968); 1.1355 should read 1.355.

This equilibrium was reached with a time constant of $\tau = 0.869$ sec, with the ground state population decaying as

$$N_t = 0.575 + 0.425 \exp\left(-\frac{t}{\tau}\right). \quad (18)$$

4. BARIUM NEUTRAL SYSTEM

4.1 Equilibrium Without Photoionization

The program was now run with input data obtained as follows:

(1) Oscillator strengths were taken from the NBS publication (Miles et al, 1969).

(2) Solar irradiance SINC(L) was taken as the value for the continuum given in the NASA Atlas (Arvesen et al, 1969), with a correction FLD(L) being included for the Fraunhofer line depth (relative to the continuum). The FLD (L) was taken from the Utrecht Atlas (Minnaert et al, 1940).

Figure 3 shows a partial term scheme for BaI, with the transitions corresponding to the brightest observed emission features being shown.

Table 1 shows the input values used. THETA(L) is the continuum solar irradiance SINC(L) expressed in photons $\text{cm}^{-2} \text{Hz}^{-1}$, and AE(L) is the Einstein A coefficient derived from the values of oscillator strength and wavelength. This model was computed with no photoionization process included. The idea was that such a model would be modified by:

(1) Removing suddenly one half of the metastable population (for each of several metastable levels in turn) after equilibrium had been reached, and observing the time taken to return to an equilibrium situation.

(2) Allowing photionizing transitions to occur, from each of the metastable levels in turn, with a rate such that a time constant for the process of about 30 sec was obtained. Then the relative intensities of the lines for each possible process could be examined. It is expected that if the recovery times found in step (1) above are short compared with the photoionization time, then there would be no detectable difference. The photoionization mechanisms were expressed for computation in terms of an oscillator strength. This concept is valid for an auto-ionizing transition, but for continuum photoionization the rate requires to be

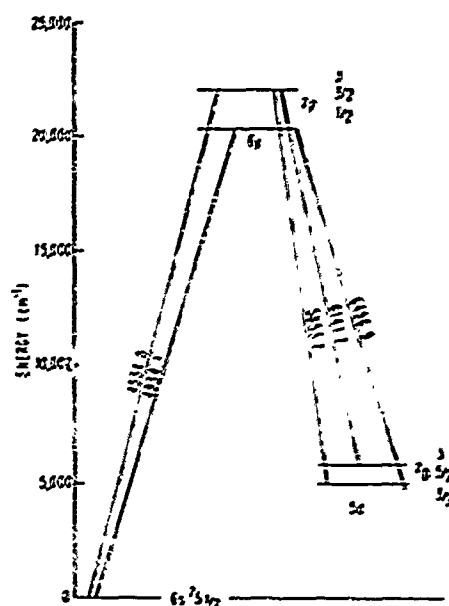


Figure 2. Barium Ion Term Diagram

Table 1. Input Data for Barium Neutral System

L	WVL(L)	NU	WL	F(L)	STNG(L)	THETA(L)	F_0(L)	AE(L)
1	2403.980	61	1	.000	.059	1.387	1.000	.615E+05
2	2414.830	60	1	.003	.050	1.419	1.000	.115E+07
3	2420.850	59	1	.007	.051	1.453	1.000	.255E+07
4	2428.170	58	1	.002	.051	1.457	1.000	.795E+06
5	2433.230	57	1	.003	.062	1.533	1.000	.943E+05
6	2439.550	55	1	.000	.053	1.535	1.000	.124E+06
7	2445.380	55	1	.002	.053	1.547	1.000	.550E+05
8	2453.120	54	1	.000	.064	1.587	1.000	.631E+05
9	2473.200	53	1	.002	.054	1.525	1.000	.584E+06
10	2500.200	52	1	.004	.054	1.589	1.000	.153E+07
11	2543.200	51	1	.012	.095	2.624	1.000	.414E+07
12	2596.640	50	1	.035	.128	3.754	1.000	.116E+08
13	2545.640	49	1	.004	.135	5.071	1.000	.112E+07
14	2702.630	47	1	.008	.248	9.222	1.000	.247E+07
15	2739.240	45	1	.003	.225	7.891	1.000	.922E+06
16	2785.290	42	1	.010	.234	8.491	1.000	.285E+07
17	3071.580	28	1	.170	.708	14.457	1.000	.402E+08
18	3501.110	22	1	.150	1.756	75.105	.943	.291E+08
19	3889.530	18	1	.010	1.050	103.745	.324	.145E+07
20	3909.910	32	2	.130	1.418	142.341	.311	.499E+08
21	3935.720	33	3	.015	.393	40.235	.909	.463E+07
22	3937.870	32	3	.025	.539	55.533	.947	.108E+08
23	3993.400	34	4	.170	1.791	191.595	.951	.555E+08
24	3995.650	33	4	.021	1.597	141.803	.903	.891E+07
25	4132.430	14	1	.019	1.750	207.403	.541	.129E+07
26	4239.560	48	8	.038	1.852	257.035	.827	.236E+08
27	4242.510	44	7	.014	2.000	255.493	.481	.781E+05
28	4264.420	39	5	.130	2.026	253.953	.757	.150E+08
29	4283.100	35	5	.250	1.842	253.053	.503	.632E+08
30	4323.000	40	7	.072	1.394	197.779	.524	.155E+08
31	4325.150	46	8	.028	1.918	205.257	.455	.716E+07
32	4332.910	39	7	.043	2.043	279.131	.777	.153E+08
33	4350.750	35	7	.253	1.715	257.129	.893	.594E+08
34	4402.540	27	7	.051	1.583	251.134	.942	.705E+08
35	4436.850	45	8	.000	1.978	254.242	.913	.103E+08
36	4431.990	25	5	1.100	2.016	254.721	.703	.125E+08
37	4457.090	43	7	.000	1.754	242.023	.954	.571E+07
38	4498.980	41	8	.280	2.315	255.105	.874	.627E+08
39	4493.640	40	8	.113	2.035	255.994	.951	.375E+08
40	4505.920	26	7	.000	2.296	251.855	.942	.106E+09
41	4523.170	39	8	.200	2.041	317.135	.951	.949E+08
42	4573.850	31	7	.021	2.216	355.038	.942	.238E+09
43	4579.560	37	8	.059	2.025	327.283	.942	.179E+07
44	4591.920	27	3	.005	2.099	341.243	.941	.155E+07
45	4593.750	30	7	.113	1.075	327.955	.831	.104E+07
46	4504.990	25	2	.018	2.047	255.713	.999	.777E+07
47	4515.920	29	6	.000	2.171	319.515	.951	.841E+07
48	4628.350	25	3	.312	2.116	312.324	.999	.625E+07
49	4573.570	27	4	.012	2.118	313.112	.975	.644E+07
50	4591.620	35	8	.333	2.095	353.335	.757	.167E+09
51	4700.430	20	7	.073	1.984	355.075	.951	.279E+08
52	4726.440	28	5	.150	2.072	357.405	.900	.699E+08
53	5535.480	9	1	1.500	1.931	511.053	.893	.116E+09
54	5777.520	26	8	1.000	1.976	507.523	1.000	.143E+09

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Only those transitions for which $BR(L) \geq 0.001 \text{ photons sec}^{-1} \text{ atom}^{-1}$ are tabulated, and their temporal behavior is characterized as follows:

Type 1: Shows "exponential" decay similar to P(1)

Type 2: Shows transient peak, similar to P(5)

Type 3: Shows exponential grow-in, similar to P(2, 3 or 4)

Type 4: Falls initially, then grows into steady value

The rate of pumping due to any transition is, of course,

$$-\frac{dP(NL)}{dt} = \frac{dP(NU)}{dt} = P(NL) \frac{\pi e^2}{mc} f_{NL,NU} \text{ THETA FLD sec}^{-1} \quad (20)$$

where $\pi e^2/mc = 0.02654$ and the values of THETA and FLD are given in Table 1.

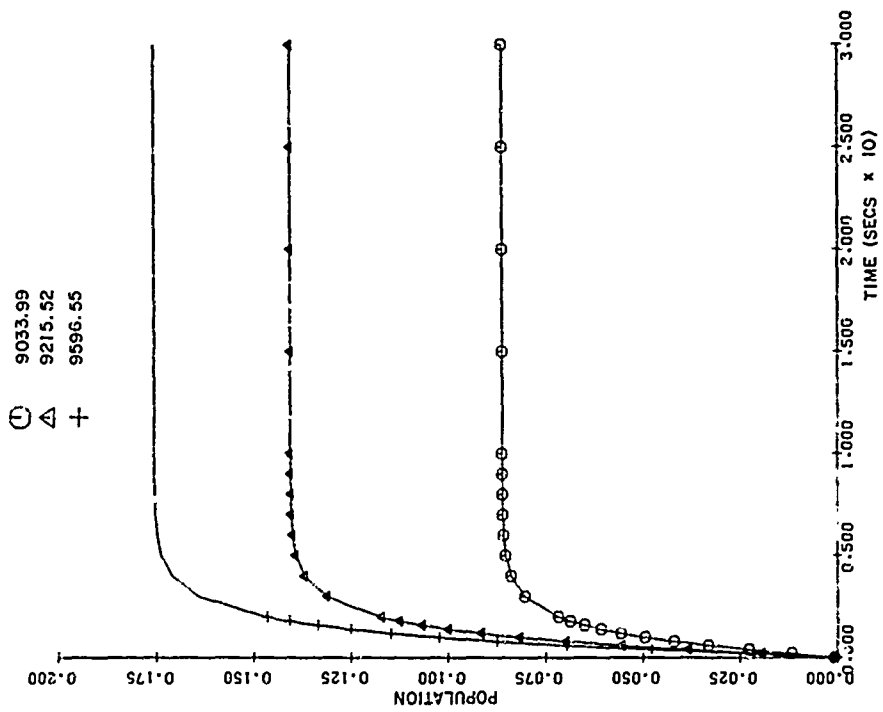
1.2 Readjustment of Equilibrium After Sudden Removal of Some Metastable Atoms

Since equilibrium was reached within 7 sec. in this run one half the 1D_2 (N=5) population was removed at 10 sec, and one half the 3D_2 (N=3) population at 20 sec. The run was terminated at 30 sec. Recovery from the first perturbation was complete within one sec for the ground state and 1D_2 metastable level, and within about 2 sec for the 3D levels. In the second case recovery for the 1D level was also complete within one sec, whereas the ground state as well as the 3D levels required about 2 sec for recovery of equilibrium populations. Since these recovery (that is, population) times are so short compared with the photoionization time constant, it may be expected that the relative line intensities will not be very sensitive to the choice of metastable level assumed to be the precursor to photoionization.

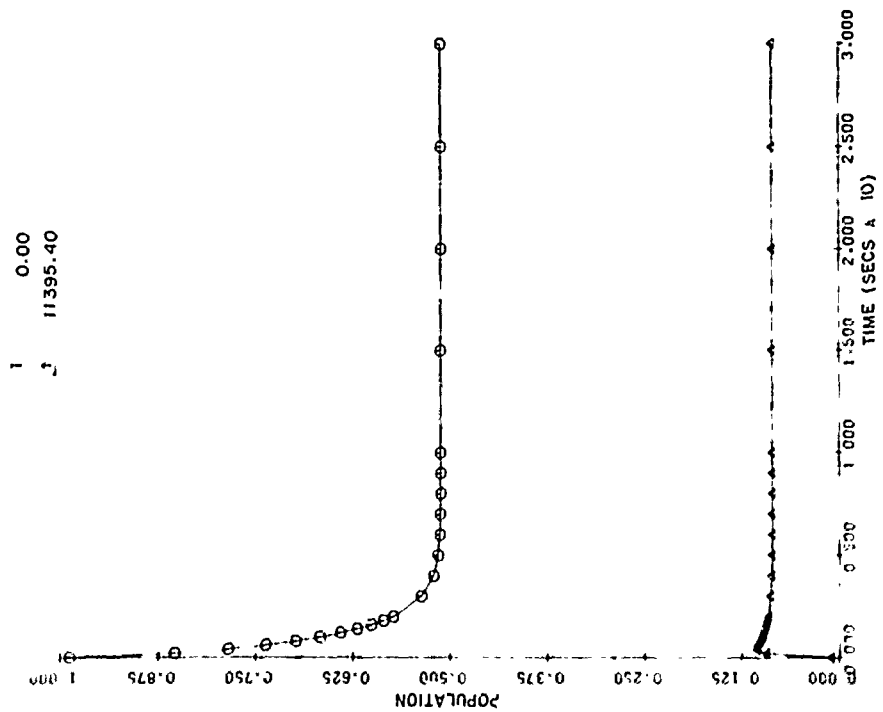
1.3 Photoionization From 1,3D Metastable Levels

Photoionization was included in the computation process by the following technique:

- (1) Add an extra energy level corresponding to the ionization limit
- (2) Increase NMAX by 1 accordingly
- (3) Allow a transition from the lower level NL concerned to the ionization limit, with the oscillator strength being chosen to yield a time constant of 30 sec. This hypothetical transition can later be equated with a photoionization continuum process, or with an autoionizing transition. This will also require a unity increase in LMAX.
- (4) Permit all downward transitions as before, up to and including (LMAX-1)



(b)



(a)

Figure 4. Populations as a Function of Time

$$P(1)_t = 0.512 + 0.394 \exp\left(-\frac{t}{\tau}\right) \quad (19)$$

where the time constant $\tau = 1.067$ sec.

At equilibrium the relative populations are:

<u>N</u>	<u>E(N)</u>	<u>P(N)</u>
1	0.0	0.512
2	9033.99	0.086
3	9215.52	0.141
4	9595.55	0.176
5	11395.40	0.085

These have been reached to within 0.001 within 7 sec.

The relative emission intensities BR(L) in units of photons per second per total barium atom are given in Table 2. As might be expected, the relative brightnesses show the same temporal behavior as corresponding energy levels. The 5535A⁰ line shows an intensity decay similar to that of the population of the ground state.

Table 2. Equilibrium Emission Line Intensities per Barium Atom, Without Ionization

L	WVL(L) Angstroms	BR(L) photon/atom sec	Type	L	WVL(L) Angstroms	BR(L) photon/atom sec	Type
12	2596	0.002	1	61	6019	0.377	3
14	2702	0.001	1	62	6063	0.800	3
16	2785	0.001	1	63	6111	1.313	3
17	3072	0.071	2	64	6342	0.405	3
18	3501	0.130	2	65	6451	0.175	3
19	3889	0.012	3	66	6482	0.636	2
20	3910	0.021	3	67	6499	1.855	3
21	3936	0.006	3	68	6527	0.986	3
22	3938	0.004	3	69	6595	0.828	3
23	3993	0.144	3	70	6675	0.401	3
24	3996	0.012	3	71	6694	0.484	3
25	4132	0.015	3	72	6868	0.102	3
29	4283	0.077	2	73	7060	2.667	3
44	4592	0.066	3	74	7120	0.532	3
46	4605	0.004	3	76	7280	1.947	3
48	4628	0.016	3	78	7418	0.064	3
52	4726	0.124	2	79	7488	0.367	3
53	5535	8.112	1	80	7672	0.832	3
56	5806	0.057	2	81	7780	0.359	3
57	5826	0.441	2	83	7911	0.128	4
58	5907	0.047	3	84	15000	0.347	1
59	5972	0.368	3	85	27750	0.048	4
60	5997	0.383	3	86	29223	0.124	3

Only those transitions for which $BR(L) \geq 0.001 \text{ photons sec}^{-1} \text{ atom}^{-1}$ are tabulated, and their temporal behavior is characterized as follows:

Type 1: Shows "exponential" decay similar to P(1)

Type 2: Shows transient peak, similar to P(5)

Type 3: Shows exponential grow-in, similar to P(2, 3 or 4)

Type 4: Falls initially, then grows into steady value

The rate of pumping due to any transition is, of course,

$$-\frac{dP(NL)}{dt} = \frac{dP(NU)}{dt} = P(NL) \frac{\pi e^2}{mc} f_{NL, NU} \text{ THETA FLD sec}^{-1} \quad (20)$$

where $\pi e^2/mc = 0.02654$ and the values of THETA and FLD are given in Table 1.

4.2 Readjustment of Equilibrium After Sudden Removal of Some Metastable Atoms

Since equilibrium was reached within 7 sec. in this run one half the 1D_2 (N=5) population was removed at 10 sec, and one half the 3D_2 (N=3) population at 20 sec. The run was terminated at 30 sec. Recovery from the first perturbation was complete within one sec for the ground state and 1D_2 metastable level, and within about 2 sec for the 3D levels. In the second case recovery for the 1D level was also complete within one sec, whereas the ground state as well as the 3D levels required about 2 sec for recovery of equilibrium populations. Since these recovery (that is, population) times are so short compared with the photoionization time constant, it may be expected that the relative line intensities will not be very sensitive to the choice of metastable level assumed to be the precursor to photoionization.

4.3 Photoionization From 1,3D Metastable Levels

Photoionization was included in the computation process by the following technique:

- (1) Add an extra energy level corresponding to the ionization limit
- (2) Increase NMAX by 1 accordingly
- (3) Allow a transition from the lower level NL concerned to the ionization limit, with the oscillator strength being chosen to yield a time constant of 30 sec. This hypothetical transition can later be equated with a photoionization continuum process, or with an autoionizing transition. This will also require a unity increase in LMAX.
- (4) Permit all downward transitions as before, up to and including (LMAX-1)

The oscillator strength was initially chosen so that

$$-\frac{dP(NL)}{P(NL)} = 0.02654 F \text{ THETA} = \frac{1}{30} \text{ sec}^{-1}. \quad (21)$$

However, it soon became apparent that F would require to be increased by $1/P(NL)$ in order to make the overall time constant of the order of 30 sec.

Table 3. Data Yielding Metastable Photoionization Time Constant of Required Magnitude

Precursor	3D_2	3D_3	1D_2
N	3	4	5
f	0.345	0.221	0.197
AE (sec $^{-1}$)	1.24(9)	1.09(9)	0.619(9)
WVL (\AA)	3046.33	3082.12	3263.09
SINC (watts m $^{-2}$ nm $^{-1}$)	0.539	0.650	1.149
THETA (phot cm $^{-2}$ sec $^{-1}$ Hz $^{-1}$)	25.59	31.961	67.044
FLD	1.000	1.000	1.000
τ (sec)	34	33	34.5
At 20 sec:			
P (1)	0.295	0.295	0.284
P (2)	0.046	0.046	0.049
P' (3)	0.074	0.075	0.080
P (4)	0.093	0.092	0.100
P (5)	0.048	0.048	0.048
P (62)	0.444	0.444	0.441

Table 3 nows the values of oscillator strength required to achieve a photo-ionization time constant of about 34 sec. Note that at 20 sec the relative values of $P(N)$ are practically indistinguishable. The rate of ionization for a bound-bound (or autoionizing) transition is given by

$$-\frac{1}{P(NL)} \frac{dP(NL)}{dt} = 0.02654 F \text{ THETA FLD sec}^{-1} \quad (22)$$

or, if it is a continuum photoionizing process the rate would be

$$\begin{aligned}
 -\frac{1}{P(N)} \frac{dP(N)}{dt} &= \int_{\lambda=0}^{\lambda_T} \sigma \theta_{\lambda} d\lambda \text{ sec}^{-1} \\
 &= \int_{\nu_T}^{\infty} \sigma \theta_{\nu} d\nu \text{ sec}^{-1}
 \end{aligned} \tag{23}$$

where σ is the photoionization cross section, and λ_T and ν_T are the threshold wavelengths and frequencies respectively.

The values of Einstein A coefficient (AE) corresponding to the required oscillator strengths are not unduly large. However, the failure by Garton (1962) to detect any autoionizing transitions from the metastable levels renders this process unlikely. It is therefore more appropriate to consider in detail the conclusions in terms of continuum-photoionization cross sections.

We can obtain an idea of the cross section involved by making either of two assumptions:

- (1) That the photoionization cross section varies slowly compared to the solar irradiance (which falls by a factor of 2 every 100 to 200 Å).
- (2) That the photoionization cross section falls off much more rapidly (with decreasing wavelength) than the solar irradiance. Then only the value at the threshold is significant. In either case we can say

$$0.02654 f = \int \sigma d\nu \approx \sigma \Delta\nu \tag{24}$$

where $\Delta\nu$ is the effective spectral width of the process determined either (a) by the solar continuum intensity as a function of wavelength, or (b) by the photoionization cross section as a function of wavelength.

If we take $\Delta\lambda = 200\text{Å}$ ($= 6 \times 10^{13}$ Hz at 3127Å), we find that

$$\begin{aligned}
 \sigma &= 4.423 \times 10^{-16} f \text{ cm}^2 \\
 &= 442 f \text{ Mb}
 \end{aligned}$$

where one megabarn (Mb) = 10^{-18} cm^2 .

Therefore if we permit photoionization to proceed from any one of the four possible metastable levels, we require a cross section of about 80 Mb. If we consider photoionization from all four metastable levels, we require a cross section of about 20 Mb and this is more in keeping with values for photoionization from the ground state measured by Hudson et al (1970). However, these values were only

maintained over a few \AA . The fact that photoionization was probably from all four metastable levels was also derived from the results of the ultra-violet-screened barium release previously reported by Best et al (1969) and Rosenberg et al (1971).

References

- Arvesen, J.C., Griffin, R.N. and Pearson, B.D. (1969) Determination of extraterrestrial solar spectral irradiance from a research aircraft, Applied Optics 8:2215-2232.
- Best, G. T. (1968) Optical Program for SECEDE III, Informal AFCKL Report.
- Best, G. T. and Rosenberg, N.W. (1969) Spectroscopic Studies of Barium Releases, paper presented at IAGA Symposium, Madrid.
- Best, G. T. and Rosenberg, N.W. (1970) Optical Study Results of SECEDE I Data, Project SECEDE, Special Report No. 12, p. 10.
- Carton, W.R.S., Parkinson, W.H. and Reeves, E.M. (1962) The absorption spectrum of shock-excited barium, Proc. Phys. Soc. 80:860-867.
- Hudson, R.D., Carter, V.L. and Young, P.A. (1970) Absorption spectrum of BaI in the region of autoionization from 2382 to 1700 Å, Physical Review A, 2:643-648.
- Miles, B.M., and Wiese, W.L. (1969) Critically Evaluated Transition Probabilities for BaI and BaII, NBS Technical Note 474.
- Minnaert, M.J.G., Mulders, G.F.W., and Houtgast, J. (1940) A Photometric Atlas of the Solar Spectrum, Schnable & Helm, Utrecht.
- Quesada, A. F. (1971) Private communication.
- Rosenberg, N.W., and Best, G. T. (1971) Chemistry of barium released at high altitudes, J. Phys. Chem. 75: 1412-8.

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Appendix A

The following printouts describe a computer program that calculates photo-equilibrium of barium. One set of printouts describes Program Relax which calculates the excitation and emission of atoms in the transient and steady state; and a second set of printouts contains Sample Data to be used.

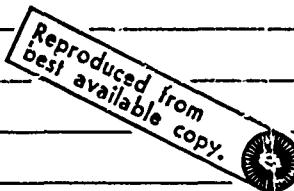
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PROGRAM RELAX

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PROGRAM RELAX(INPUT,OUTPUT,TAPE5=INPUT,TAPE3=OUTPUT,TAPE19,TAPE2,
1TAPE8,TAPE9)
C
C THIS PROGRAM CALCULATES THE EXCITATION AND EMISSION OF ATOMS
C IN THE TRANSIENT AND STEADY STATE.
C
C INTEGER 3
COMMON E(100),G(100),P(100),PP(100)
COMMON THETA(100),AE(100),BR(100),RAE(100),RAT(100)
COMMON ALV(100),NU(100),NL(100),F(100),SINC(100),FLD(100)
COMMON TIT(200),BRT(200),PT(200)
DIMENSION YLABL(3),TITL(9),XL(2),YL(2), ASEL(3),YLABEL(3)
DIMENSION INDX(101),INDY(101),IPL(12),ITL(8),SCALE(10),ISCL(3)
C
C SET CONSTANTS.
C
C IND=0
C K=0
C KK=0
C DELTC=0.01
C TIME=0.0
C WRITE(5,10)
10 FORMAT (11,/)
C
C NMN IS LOWEST VALUE OF NJ WHICH SHOULD BE EMPTY AFTER EMISSION.
C
C NMN=9
C
C READ IN THE NUMBER OF ENERGY LEVELS, THE NUMBER OF POSSIBLE
C TRANSITIONS AND THE NUMBER OF SECONDS THE REACTION SHOULD GO.
C
C READ(5,20) NMAX,LMAX,FTIME
20 FORMAT (2I5,F3.0)
C DO 11 N=2,NMAX
C P(N)=0.0
11 CONTINUE
C P(1)=1.0
C
C READ THE ENERGY LEVELS AND THE G FACTOR.
C INPUT E(N) IN CM-1, G IS STATISTICAL WEIGHT.
C
C READ(5,30) (E(N),G(N),N=1,NMAX)
30 FORMAT (5X,=10.0,I5)
C
C READ THE WAVELENGTH OF THE TRANSITIONS, THE UPPER AND LOWER ENERGY
C LEVELS, F, SINC, AND FLD.
C WVL IS ANGSTROMS IN AIR IF ALVAC .GE. 2450A.
C WVL IS ANGSTROMS IN VAC IF ALVAC .LT. 2450A.
C SINC IS SOLAR INTENSITY IN CONTINUUM IN WATTS M**2 NM-1
C (APPL. OPT. 9,345(1970))
C FLD IS FRAUNHOFER LINE DEPTH.

```



```

C      FLD IS 1.000 FOR NO ABSORPTION.
C
C      READ(5,40) (HVL(L),NU(L),NLL(L),F(L),SINC(L),FLD(L),
+L=1,LMAX)
40      FORMAT (5X,F10.0,2I5,E10.0,2F10.0)
C
C      CALCULATE THE VALUES OF THETA.
C      THETA IS SOLAR IRRADIANCE AT MEAN EARTH DISTANCE IN PHOTONS CM**2
C      SEC-1 4Z-1 IN SOLAR CONTINUUM.
C
C      DO 21 L=1,LMAX
C      THETA(L)=SINC(L)*1679.4*((HVL(L)*1.0E-04)**3)
21      CONTINUE
C
C      CHECK THAT THE ENERGY DIFFERENCES ARE CONSISTENT WITH THE
C      WAVELENGTHS WHICH WERE PREVIOUSLY READ.
C
C      DO 31 L=1,LMAX
C      NUL=NU(L)
C      NLL=NLL(L)
C      HLVAC=1.0E08/(E(NUL)-E(NLL))
C      IF(HLVAC.LT.2460.) HLD=HLVAC-HVL(L)
C      IF(HLVAC.GE.2460.) HLD=(HLVAC-0.075)/1.000265
C      IF(HLVAC.GE.2460.) HLD=HLVAC-HVL(L)
C      IF(ABS(HLD).GT.0.25) GO TO 5
C      GO TO 31
5      WRITE(6,50) L,HVL(L),NUL,NLL,E(NUL),E(NLL)
50      FORMAT (* THE FOLLOWING DATA IS NOT CONSISTENT,*/,
+* L=*I5,* HVL(L)=*F8.2,* NU(L)=*I3,* NLL(L)=*I3,
+* E(NUL)=*F8.1,* E(NLL)=*F8.1)
C      IND=1
31      CONTINUE
C
C      EXIT IF ANY VALUE IS NOT CONSISTENT.
C
C      IF(IND.EQ.1) STOP
C
C      CALCULATE WAVELENGTHS IN MICRONS, AND EINSTEIN COEFFICIENTS.
C
C      DO 91 L=1,LMAX
C      NUL=NU(L)
C      NLL=NLL(L)
C      HLM=1.0E+4/(E(NUL)-E(NLL))
C      AE(L)=(FLOAT(G(NLL))/FLOAT(G(NUL)))*0.6598E+8*(L)/(HLM**2)
91      CONTINUE
C      WRITE(6,110)
110     FORMAT (4X,*L*3X*HVL(L)*3X*NU*2X*NLL*6X*F(L)*3X
+*SINC(L)*2X*THETA(L)*4X*FLD(L)*4X*AE(L)*
C      WRITE(6,200) (L,HVL(L),NU(L),NLL(L),F(L),SINC(L),THETA(L),
+FLD(L),AE(L),L=1,LMAX)
200     FORMAT (I5,F10.3,2I4,4F10.3,E10.3)

```

```

C
C CALCULATE THE RAE COEFFICIENTS WHICH DETERMINE HOW THE LEVELS
C WILL BE DEPLETED BY EACH EMISSION FROM THE LEVEL.
C
DO 101 N=1, NMAX
SUM=0.0
DO 111 L=1, LMAX
IF(NJ(L).EQ.0) SUM=SUM+RAE(L)
111 CONTINUE
DEC=SUM*DELTC
IF(DEC.LT.10.0.AND.N.GE.NMIN) WRITE(5,80) N
80 FORMAT (/' LEVEL'13' HAS NOT COMPLETELY EMPTIED')
DO 121 L=1, LMAX
IF(NJ(L).EQ.0) RAE(L)=RAE(L)/SUM
121 CONTINUE
101 CONTINUE
C
C START LOOP WHICH CALCULATES THE PUMPING OF STATES AND THE EMISSION
C EVERY DELED SECONDS.
C
55 TIME=TIME+DELTC
DO 61 N=1, NMAX
PP(N)=0.0
31 CONTINUE
K=K+1
C
C CALCULATE RATE OF PUMPING AT EACH LEVEL.
C
DO 41 L=1, LMAX
NJL=NJ(L)
NLL=NL(L)
RAT(L)=0.02554*PP(NLL)*F(L)*THETA(L)*ED(L)*DELTC
PP(NJL)=PP(NJL)+RAT(L)
PP(NLL)=PP(NLL)-RAT(L)
41 CONTINUE
C
C CALCULATE NEW POPULATIONS.
C
DO 71 V=1, VMAX
P(V)=P(N)+PP(N)
PP(N)=0.0
71 CONTINUE
C
C CALCULATE EMISSIONS FROM EACH LEVEL.
C
LMAX1=LMAX-1
DO 51 L=1, LMAX1
NJL=NU(L)
NL=NL(L)
3 BR= PHOTONS/SEC.
RATE=P(NJL)*RAE(L)

```



```

      BR(L)=RATE/DELTC
      P(INH)=P(L)+RATE
      P(NUH)=P(L)-RATE
52    CONTINUE
53
54    CALCULATE THE POPULATIONS.
55
56    DO 51 N=1,NMAX
57      P(T)=P(N)+PP(N)
58      P(NU)=0.0
59
60    CHECK THAT ALL LEVELS GREATER THAN THIN HAVE EXPIRED.
61
62    IF (INSE.XITV.AND.P(N).GT.0.JO(51.4V).V.NE.NMAX) GO TO 15
63    GO TO 51
64
65    WRITE(6,99) N
66    FORMAT (//,13,' HAS NOT EXPIRED')
67    CONTINUE
68
69    CHECK IF THE POPULATION VALUES AND BRIGHTNESSES SHOULD BE
70    PRINTED AT THIS TIME.
71
72    IF(K.EQ.1) GO TO 65
73    IF((K/20)*23.NE.K) GO TO 55
74    IF(TIME.-E.2.0) GO TO 65
75    IF((K/100)*100.NE.K) GO TO 55
76    IF(TIME.-E.10.0) GO TO 65
77    CONTINUE
78    KK=KK+1
79
80    WRITE DATA ON A TAPE FOR STORAGE.
81
82    WRITE(2) TIME,(BR(L),P(L),L=1,LMAX)
83    WRITE(5,76) TIME
84    FORMAT (//,30X,'TIME =',F7.3/)
85    WRITE(5,133)
86    FORMAT (//,44X,'N*6X*E(N)*5X*P(N)*')
87    WRITE(5,53) N,E(N),P(N),N=1,NMIN,NMAX,E(NMAX),P(NMAX)
88    FORMAT (4X,15,2F10.3)
89    WRITE(5,149)
90    FORMAT (//,34X,'L*4X*VL(L)*8X*RATE(L)*3X*NU*3X*NL*10X-BR(L)*')
91    WRITE(5,120) (L,NVL(L),RAT(L),NJ(L),VL(L),BR(L),L=1,LMAX)
92    FORMAT (33X,15,F10.3,E15.3,2I5,F15.3)
93
94    CHECK IF WE HAVE ALLOWED THE CALCULATION TO GO TO COMPLETION.
95
96    IF(TIME.-I.FTIME) GO TO 55
97    ENDFILE 2
98    REWIND 2
99
100    NOTE: The remaining portion of the program sorts the data so that it can
101    be plotted. This portion of the program is particular for the CDC6600, and
102    subroutine PLOT V is a plotting subroutine written by the author for the
103    CalComp Platter.
104
105    SET JP CONSTANTS FOR PLOTTING.

```

```

DATA X_/0.3,30.0/
YL(1)=0.0
XS=5.0
DATA X_LABEL_/304          TIME (SECS)      /
DATA Y_LABEL_/304          BRIGHTNESS        /
DATA Y_LABEL_/304          POPULATION         /
DATA (TITLE(I),I=2,8,2)/4*104 (SY-1)      /
DATA (TITLE(I),I=2,8,2)/4*104WAVELENGTHS /
DATA EN/104WAVELENGTH /

C
C OPEN MASS STORAGE FILE ON UNIT 8 FOR POPULATIONS, AND ON UNIT 9
C FOR BRIGHTNESSES, AND STORE THE DATA ON TAPE 2 IN THE PROPER FILES
C
      CALL OPENMS(8,INDX,101,0)
      CALL OPENMS(9,INDY,101,0)
      DO 131 L=1,LMAX
      DO 151 K=1,KK
      READ(2) TIT(L),(SINC(M),FJ(M),M=1,LMAX)
      BRT(LL)=SINC(LL)
      PT(LL)=FJ(LL)
151 CONTINUE
      CALL WRITMS(3,BRT,KK,L)
      IF(L.GT.NMAX) GO TO 135
      CALL WRITMS(5,PT,KK,L)
135 REWIND 2
131 CONTINUE
      IND=0
      DATA SCALE/2.5,1.0,0.75,0.50,0.25,0.125,0.05,0.025,0.010,0.005/

C
C READ THE CODE FOR THE TYPE OF DATA TO BE PLOTTED,THE NUMBER
C OF SPECTRAL LINES OR ENERGY LEVELS, THE CODE FOR THE SPECTRAL
C LINE OR ENERGY LEVEL AND THE SCALE CODE.
C
25 READ(5,100) ENG,J,(IPL(I),I=1,4),ISCL(1),(IPL(I),I=5,8),
1ISCL(2),(IPL(I),I=9,12),ISCL(3)
100 FORMAT (A10,I10,15I4)
      IS=0

C
C CHECK IF ALL THE CASES HAVE BEEN PLOTTED.
C
      IF(J.GT.12) GO TO 75

C
C CHECK IF WE ARE GOING TO PLOT ENERGY LEVELS OR WAVELENGTHS.
C
      IU=8
      IF(ENG.EQ.24) IU=9
      DO 141 I=1,J,4
      ND=3
      I4=I+3
      IF(IND.EQ.0) ND=1

```

```

IF(IU.EQ.9) GO TO 35
IV=0
DO 171 II=I,I4
IP=IPL(II)
IV=IV+1
IF(IP.EQ.0) GO TO 85
IF(II.GT.J) GO TO 85
C
C   PREPARE TITLE AND INITIALIZE PLOTTER.
C
IF(IJ.EQ.8) ENCODE(10,150,TITL(2*IV-1)) E(IP)
GO TO 171
85 TITL(2*IV-1)=10H
171 CONTINUE
IS=IS+1
ISS=ISCL(ISS)
YL(2)=8.0*SCALE(ISS)-0.001
YS=SCALE(ISS)
CALL PLOTV(NJ,XL,XS,YL,YS,2,33,-1,-8),TITL ,XLABEL,YLABL ,8.5,11.)
GO TO 45
35 CONTINUE
IV=0
DO 151 II=I,I4
IP=IPL(II)
IV=IV+1
IF(II.GT.J) GO TO 95
IF(IP.EQ.0) GO TO 95
IF(IJ.EQ.9) ENCODE(10,150,TITLE(2*IV-1)) HWL(IP)
150 FORMAT (1X,F8.2,1X)
GO TO 161
95 TITLE(2*IV-1)=104
161 CONTINUE
IS=IS+1
ISS=ISCL(ISS)
YL(2)=8.0*SCALE(ISS)-0.001
YS=SCALE(ISS)
CALL PLOTV(NJ,XL,XS,YL,YS,2,33,-1,-8),TITLE,XLABEL,YLABEL,8.5,11.)
C
C   PLOT CURVES.
C
C
45 DO 141 II=I,I4
IF(II.GT.J) GO TO 141
IF(IPL(II).EQ.0) GO TO 141
CALL READMS(IJ,PT,KK,IPL(II))
NO=2
N=II-I+1
CALL PLOTV(NJ,TIM,XS , PT,YS ,KK,N,1,-80,TITL ,XLABEL,YLABEL,
18.5,11.)
IND=1
141 CONTINUE
GO TO 25
75 CALL PLOTV(4)
STOP
END
MARK ENCOUNTERED

```

SAMPLE DATA

52	37	23.
1	0.000	1
2	9033.33	3
3	9215.52	5
4	9595.55	7
5	11395.4	5
6	12266.0	1
7	12535.5	3
8	13514.7	5
9	16060.3	3
10	22054.7	5
11	22947.4	7
12	23074.4	5
13	23757.1	9
14	24192.1	3
15	24531.5	5
16	24979.9	7
17	25642.2	1
18	25704.1	3
19	25956.5	5
20	26160.3	3
21	26815.3	7
22	28554.3	3
23	30743.5	1
24	30750.7	5
25	30815.5	3
26	30818.1	7
27	30987.3	5
28	32547.1	3
29	33905.3	3
30	34370.8	1
31	34493.9	1
32	34602.8	5
33	34616.7	7
34	34630.8	9
35	34736.4	7
36	34823.4	3
37	35344.4	5
38	35616.9	5
39	35709.3	3
40	35762.2	5
41	35785.3	7
42	35892.5	3
43	35894.3	7
44	36200.4	5
45	36495.8	3
46	36628.9	7
47	36990.0	3
48	37095.5	3
49	37774.5	3
50	38499.9	3

51	39388.7	3					
52	39984.8	3					
53	40421.23	3					
54	40764.4	3					
55	40893.4	3					
56	40991.2	3					
57	41096.8	3					
58	41183.3	3					
59	41307.8	3					
60	41410.8	3					
61	41494.1	3					
62	42032.4	1					
1	2409.93	51	1	1.6 E-04	.059	1.000	
2	2414.83	52	1	3.0 E-03	.060	1.000	
3	2420.85	59	1	5.7 E-03	.061	1.000	
4	2428.17	58	1	2.1 E-03	.061	1.000	
5	2433.28	57	1	2.5 E-03	.062	1.000	
6	2439.55	56	1	3.3 E-04	.063	1.000	
7	2445.38	55	1	1.5 E-03	.063	1.000	
8	2453.12	54	1	1.7 E-04	.064	1.000	
9	2473.20	53	1	1.6 E-03	.064	1.000	
10	2500.2	52	1	4.3 E-03	.064	1.000	
11	2543.2	51	1	1.2 E-02	0.095	1.000	
12	2595.54	50	1	3.5 E-02	0.128	1.000	
13	2646.54	49	1	3.5 E-03	0.195	1.000	
14	2702.53	47	1	9.1 E-03	0.248	1.000	
15	2739.24	45	1	3.1 E-03	0.226	1.000	
16	2785.28	42	1	9.9 E-03	0.234	1.000	
17	3071.58	28	1	1.7 E-01	0.708	1.000	
18	3501.11	22	1	1.6 E-01	1.356	0.343	
19	3889.33	18	1	1.0 E-02	1.350	0.324	
20	3909.91	32	2	1.9 E-01	1.418	0.311	
21	3935.72	33	3	1.5 E-02	0.393	0.309	
22	3937.87	32	3	2.5 E-02	0.539	0.347	
23	3993.40	34	4	1.7 E-01	1.791	0.351	
24	3995.55	33	4	2.1 E-02	1.597	0.303	
25	4132.43	14	1	9.9 E-03	1.750	0.541	
26	4239.55	46	8	3.8 E-02	1.552	0.527	
27	4242.61	44	7	3.5 E-03	2.300	0.481	
28	4264.42	39	6	1.3 E-01	2.326	0.757	
29	4283.10	35	5	2.5 E-01	1.342	0.563	
30	4323.00	40	7	7.2 E-02	1.384	0.524	
31	4325.15	46	8	2.8 E-02	1.518	0.456	
32	4332.91	39	7	4.3 E-02	2.343	0.777	
33	4350.33	38	7	2.8 E-01	1.715	0.883	
34	4402.54	37	7	3.4 E-01	1.583	0.342	
35	4406.85	44	8	3.0 E-02	1.378	0.913	
36	4431.89	36	6	1.1 E-00	2.316	0.709	
37	4467.09	43	8	2.8 E-02	1.354	0.854	
38	4488.98	41	8	1.8 E-01	2.015	0.874	
39	4493.64	40	8	1.1 E-01	2.308	0.951	

40	4505.92	36	7	3.2	E-01	2.290	0.342								
41	4523.17	38	8	2.9	E-01	2.141	0.351								
42	4573.55	31	7	3.1	E-01	2.216	0.342								
43	4579.64	37	3	5.6	E-01	2.329	0.342								
44	4591.82	27	3	5.2	E-03	2.398	0.381								
45	4599.75	30	7	1.1	E-01	1.375	0.331								
46	4604.93	23	2	5.2	E-03	2.047	0.599								
47	4619.92	29	5	9.0	E-02	2.171	0.351								
48	4628.33	25	3	1.2	E-02	2.116	0.390								
49	4673.62	27	4	1.5	E-03	2.118	0.376								
50	4631.52	36	8	3.3	E-01	2.395	0.757								
51	4700.43	29	7	7.9	E-02	1.384	0.351								
52	4725.44	28	5	1.4	E-01	2.372	0.390								
53	5535.43	9	1	1.59	E-00	1.331	0.580								
54	5777.52	26	8	1.0	E-08	1.376	1.000								
55	5800.23	24	8	2.4	E-01	1.376	1.100								
56	5805.69	21	4	2.0	E-02	1.331	0.380								
57	5825.30	22	5	3.0	E-01	1.341	1.100								
58	5907.54	19	2	3.1	E-02	1.311	1.100								
59	5971.70	19	3	1.5	E-01	1.393	1.100								
60	5997.09	18	2	2.5	E-01	1.762	1.900								
61	6019.47	17	2	2.5	E-01	1.745	0.390								
62	6053.12	18	3	3.2	E-01	1.345	1.100								
63	6110.79	19	4	4.0	E-01	1.325	1.000								
64	6341.68	16	3	1.6	E-01	1.575	1.000								
65	6450.65	15	2	1.1	E-01	1.522	0.387								
66	6482.91	21	5	3.9	E-01	1.527	0.371								
67	6498.75	16	4	5.5	E-01	1.564	0.390								
68	6527.31	15	3	3.8	E-01	1.545	0.322								
69	6595.33	14	2	4.7	E-01	1.561	0.390								
70	6675.27	14	3	1.4	E-01	1.526	1.000								
71	6693.84	15	4	1.4	E-01	1.578	1.100								
72	6865.69	19	5	5.5	E-02	1.489	1.000								
73	7059.94	13	4	5.8	E-01	1.450	0.381								
74	7120.33	12	2	2.7	E-01	1.438	0.390								
75	7195.24	20	6	5.6	E-01	1.373	0.380								
76	7280.30	11	3	5.9	E-01	1.366	1.000								
77	7392.41	20	7	4.1	E-01	1.322	1.100								
78	7417.53	12	4	1.5	E-02	1.304	0.385								
79	7488.08	11	4	8.4	E-02	1.312	1.000								
80	7672.09	10	2	4.5	E-01	1.241	0.301								
81	7780.48	10	3	1.2	E-01	1.218	0.733								
82	7905.75	20	8	3.5	E-01	1.178	1.000								
83	7911.33	7	1	9.94	E-03	1.171	1.000								
84	15000.00	9	5	1.00	E-01	0.297	1.000								
85	27750.22	7	2	1.54	E-02	0.335	1.000								
86	29222.72	7	3	2.63	E-02	0.330	1.000								
87	3263.09	52	5	0.1970		1.149	1.100								
LEVFLS		11	01	05	52	00	05	02	03	04	00	08	06	07	08
HAVELENGTH		12	17	19	53	25	08	29	57	65	72	06	54	55	20
HAVELENGTH		08	63	61	54	73	04	30	71	67	50	05			